Propyl tert-butyl ether

Other names:	2-methyl-2-propoxypropane
	Propane, 2-methyl-2-propoxy-
	propyl 1,1-dimethylethyl ether
	tert-butyl propyl ether
Inchi:	InChI=1S/C7H16O/c1-5-6-8-7(2,3)4/h5-6H2,1-4H3
InchiKey:	FITVQUMLGWRKKG-UHFFFAOYSA-N
Formula:	C7H16O
SMILES:	CCCOC(C)(C)C
Mol. weight [g/mol]:	116.20
CAS:	29072-93-3

Physical Properties

Property code	Value	Unit	Source
gf	-94.10	kJ/mol	Joback Method
hf	-328.78	kJ/mol	Joback Method
hfus	7.66	kJ/mol	Joback Method
hvap	38.30	kJ/mol	NIST Webbook
hvap	37.20 ± 0.60	kJ/mol	NIST Webbook
hvap	36.60 ± 0.20	kJ/mol	NIST Webbook
log10ws	-1.95		Crippen Method
logp	2.212		Crippen Method
mcvol	115.360	ml/mol	McGowan Method
pc	2805.41	kPa	Joback Method
rinpol	710.00		NIST Webbook
rinpol	704.40		NIST Webbook
rinpol	704.40		NIST Webbook
rinpol	704.00		NIST Webbook
tb	370.60 ± 0.30	K	NIST Webbook
tc	553.95	K	Joback Method
tf	193.30	K	Joback Method
vc	0.434	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	289.71	J/mol×K	553.95	Joback Method
cpg	219.51	J/mol×K	378.75	Joback Method
cpg	232.48	J/mol×K	407.95	Joback Method
cpg	244.93	J/mol×K	437.15	Joback Method
cpg	256.86	J/mol×K	466.35	Joback Method
cpg	268.29	J/mol×K	495.55	Joback Method
cpg	279.24	J/mol×K	524.75	Joback Method
dvisc	0.0002529	Pa×s	378.75	Joback Method
dvisc	0.0073885	Pa×s	193.30	Joback Method
dvisc	0.0028572	Pa×s	224.21	Joback Method
dvisc	0.0013910	Pa×s	255.12	Joback Method
dvisc	0.0007911	Pa×s	286.02	Joback Method
dvisc	0.0005023	Pa×s	316.93	Joback Method
dvisc	0.0003458	Pa×s	347.84	Joback Method
hfust	9.87	kJ/mol	179.60	NIST Webbook

Sources

Thermodynamic Analysis of the Experimental Equilibria for the Liquid-Phase Etherification of Isobutene with C1 to C4 Linear Primary Alcohols:	https://www.doi.org/10.1021/acs.jced.5b00557
Joback Method:	https://en.wikipedia.org/wiki/Joback_method
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C29072933&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws

Legend

cpg:	Ideal gas heat capacity
dvisc:	Dynamic viscosity
gf:	Standard Gibbs free energy of formation
hf:	Enthalpy of formation at standard conditions
hfus:	Enthalpy of fusion at standard conditions
hfust:	Enthalpy of fusion at a given temperature
hvap:	Enthalpy of vaporization at standard conditions
log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume

pc:	Critical Pressure
rinpol:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume